

Lattice gas model for fragmentation: From Argon on Scandium to Gold on Gold

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Abstract

The recent fragmentation data for central collisions of Gold on Gold are even qualitatively different from those for central collisions of Argon on Scandium. The latter can be fitted with a lattice gas model calculation. Effort is made to understand why the model fails for Gold on Gold. The calculation suggests that the large Coulomb interaction which is operative for the larger system is responsible for this discrepancy. This is demonstrated by mapping the lattice gas model to a molecular dynamics calculation for disassembly. This mapping is quite faithful for Argon on Scandium but deviates strongly for Gold on Gold. The molecular dynamics calculation for disassembly reproduces the characteristics of the fragmentation data for both Gold on Gold and Argon on Scandium.

I. INTRODUCTION

Recently we proposed a lattice gas model which was used to calculate mass distributions seen in heavy ion collisions at intermediate energy [1,2]. There are several features of this model that are attractive. The model can be used to study liquid-gas phase transition in mean-field theory and thus has links with Skyrme model studies of phase transitions. But the model can also be used to obtain cluster distributions and in this respect has close ties with percolation model of fragmentation which has been used [3,4] with success in theoretical studies of heavy ion collisions. However, the lattice gas model has both kinetic energy and interactions, thus the scope of the model goes beyond that of standard percolation model.

The model was used to fit the data obtained in Michigan State University for central collisions of Ar on Sc [5,6]. There are several features of the model that are quite general and are also seen in experiments. First of all, there is a region of beam energy where the yield of $Y(A)$ of fragments as a function of the mass number A of the fragment obeys a power law first noted in pioneering experiments by the Purdue group [7]. This feature emerges in theoretical calculations also. In the lattice gas model the input in a calculation is the temperature and on general grounds the higher the beam energy, the higher the temperature. In the lattice gas model there is a temperature at which a power law will emerge. If in the vicinity of this critical temperature the mass distribution is fitted by a power law whose exponent is denoted by τ then we expect to see a minimum in the extracted value of τ at the critical temperature. It is difficult to miss a minimum in τ in percolation type approach and also in the lattice gas approach. This minimum was seen in the Michigan experiment and was found in the calculation of [1,2] at the experimental beam energy. Such a minimum in the value of τ has also been seen in a recent experiment at Chalk River Nuclear Laboratories [8] and the fit with a lattice gas model calculation is quite pleasing [9]. Thus it seems that the lattice gas model simulates the fragmentation of nuclear matter reasonably well at least for medium mass collisions.

Very recent data for Au on Au central collisions [10] are at variance with these general

expectations. In the range of beam energy 35 MeV/nucleon to 100 MeV/nucleon no minimum in τ was seen. Since this is now a much bigger system and phase transition effects should become more pronounced as we go to bigger systems, this absence of a minimum in τ seems to cast serious doubts about the validity of the model. The other remarkable result is that at 35 MeV/nucleon of beam energy the deduced value of τ is much below 2; it is 1.25. Such a low value of τ will be difficult to obtain in the lattice gas model even including shape effects as discussed in [11]. Thus if we apply the lattice gas model as proposed in [1] and [2] the calculation will not fit the data for the central collisions of Au on Au.

The present work started as an effort to understand this puzzle. Between Ar on Sc and Au on Au the main difference is not only the sizes but also that in the latter case there is a huge Coulomb field whereas presumably in the former case the Coulomb field is merely a minor perturbation. Now the lattice gas model is a model of nearest neighbour interactions. The Coulomb field is a long range force and thus is not amenable to lattice gas type of approximation. One way to investigate the effect of the Coulomb field would be to try to add the effect of Coulomb force in the lattice gas type of approach but we could find no obvious way of doing that. We had provided a prescription, based on simple physical reasoning, to decide if two nucleons occupying neighbouring sites, form part of the same cluster or not. When in addition there is a long range force that distinguishes very strongly between neutrons and protons, this criterion clearly needs to be modified. There is no simple way of knowing how the modification should be made. Hence to find what effects a strong Coulomb field may have on a lattice gas model prediction, we need to try a somewhat convoluted approach. We first try to map the lattice gas model calculation to a molecular dynamics type calculation, both first done without any Coulomb interaction. If the calculations match quite faithfully then we can study the effects of the Coulomb interaction by adding that to the molecular dynamics calculation. Hopefully we will find that for Ar on Sc the Coulomb interaction does not severely change results and that the changes are very significant for the case Au on Au. We do not do an *ab initio* molecular dynamics calculation but only use it for disassembly from a thermally equilibrated source. The starting point

of the lattice gas model is that matter has equilibrated at some temperature T . There are n nucleons and N lattice sites ($N > n$). Which particular lattice sites are occupied are entirely dictated by statistical mechanics. Each cubic lattice has a size $1.0/\rho_0 = 6.25 \text{ fm}^3$ and can, at most, be occupied by a single nucleon. This starting point of calculation will not be questioned in the present work but we will use two different prescriptions for obtaining the yield $Y(A)$ against A . One of these two is our old prescription [1,2]. Nucleons occupying neighbouring sites will have attractive interactions $-\epsilon$ and are considered to be part of the same cluster provided the kinetic energy of relative motion of these two nucleons does not overcome their binding. This is enough information to deduce the yield $Y(A)$. In the alternative prescription that we will carry out here we fall back upon a more standard many body calculation. At the starting point when the nucleons have been initialised at their lattice sites and have their initial momenta, we will switch to a molecular dynamics calculation in which we will let the system evolve according to standard classical mechanics. Nucleons which stay together after arbitrarily long time are part of the same cluster. After a sufficiently long time the mass distribution is obtained. This can now be compared with lattice gas model predictions. Obviously for this test to be made with the lattice gas model we should choose for disassembly by molecular dynamics an interaction which suits the lattice gas model the best. The potential should be deepest with the value $-\epsilon$ when the two nucleons are $r_0 = 1.842 \text{ fm}$ apart and should fall to 0 before $\sqrt{2} \times 1.842 \text{ fm}$ (the next nearest neighbour interaction is zero in the lattice gas model). For distance less than 1.842 fm the potential should quickly become repulsive (two nucleons can not occupy the same site). If the two prescriptions match for the yield $Y(A)$, then we have linked the lattice gas model prediction for the yield $Y(A)$ against A to a more well-known and better understood molecular dynamics approach. Considering that the lattice gas model can be easily linked with percolation model this in itself is quite interesting; we have provided a connection between percolation model results and molecular dynamics which seem to address totally different scenario to start out with. Secondly, in case the two results match in the absence of a Coulomb field, we can, in the molecular dynamics approach find out what a large Coulomb

field, which can not be incorporated in the lattice gas model, can do to the yield $Y(A)$ since the Coulomb interaction is easily incorporated in molecular dynamics calculations. We will give the necessary details of these two calculations in the next section.

We reiterate that our objective is not a molecular dynamics calculation as such [12,13]; we use disassembly by molecular dynamics with a nuclear force that produces results similar to those of lattice gas model. This work is focussed towards one question only: we ask why the lattice gas model which worked reasonably well for Ar on Sc fails in the case of Au on Au and if we can relate this failure to the large Coulomb field which is present in the second case. We note also that the Coulomb interaction can be incorporated in microcanonical models [14,15].

II. DETAILS OF CALCULATION

Motivation and details of the lattice gas model are given in [1] and [2]. For completeness some of these details are provided in this section. The calculations all require numerical simulation involving Monte-Carlo. The starting point of all our calculations is this. For a system of n nucleons we consider N lattice sites where $N > n$. N is a parameter chosen in [1,2] by requiring the best fit. The quantity $N/n = \rho_0/\rho$ where ρ_0 is the normal density and ρ is the so called freeze-out density. It will be seen in the following that in the lattice gas calculation for fragments this freeze-out density is the actual density at which all clusters are calculated. For the molecular dynamics calculation that we will perform ρ is the density at which the initialisation is done according to prescription of equilibrium statistical mechanics. We then let the system evolve in time and the cluster distributions are calculated much later. Thus strictly speaking ρ is not a freeze-out density for molecular dynamics calculation but merely defines the starting point for time evolution. However since classical evolution of a many particle system is entirely deterministic, the initialisation does have in it all the information of the asymptotic cluster distribution. We will continue to call ρ the freeze-out density.

For initialisation, we assume that the nuclear part of the interaction is simply $-\epsilon$ between nearest neighbours and zero otherwise. To begin a calculation we have to determine which of the sites nucleons occupy and what their momenta are. The two samplings can be done independently of each other. In a percolation model the N sites would be occupied with an occupation probability $p = n/N$ by n nucleons in which each site has an equal *a priori* probability. Because of interactions this is somewhat more complicated in our case. Let us assume we are handling the case where we will take into account the Coulomb interaction explicitly in the initialisation. Starting with all lattice sites empty, the first nucleon (a proton or a neutron as dictated by a Monte-Carlo decision) is put at a site at random. If this first nucleon is a neutron then the probability of occupation of its nearest neighbours is proportional to $\exp(\beta\epsilon)$ whereas all other sites have an occupation probability proportional to 1. As usual, β is the inverse of kT . These probabilities are now used to put in the second nucleon. If the first nucleon was a proton and the second one is a neutron then again the same probability of occupation will be used. But if the second nucleon is a proton also then the above occupation probabilities are changed to proportional to $\exp(\beta\epsilon - \beta u_c)$ for the nearest neighbours and proportional to $\exp(-\beta u_c)$ for the other sites where $u_c = e^2/r$, r being the appropriate distance between the two lattice sites. It is obvious how to repeat this procedure till the prescribed number of protons and neutrons are obtained. It is also obvious how to obtain the initial configuration when the Coulomb force is not explicitly included. In that case the prescription is identical with what was used in [1] and [2].

We do some initialisations where we take the Coulomb interaction explicitly and some initialisations when the Coulomb interaction is not taken into account separately. The nuclear part is always characterised by a strength $-\epsilon$ which is the nearest neighbour type and has the same value irrespective of the isotopic spin. For a given nucleus the value of ϵ is lower for the case when the Coulomb interaction is not explicitly added. This is required by demanding that the same binding energy is obtained in both the prescriptions. In the other case when the Coulomb interaction is explicitly included the nuclear part of the interaction will lead to a larger binding which will be somewhat compensated by the repulsive Coulomb

part. For the cases dealt with here ϵ changes by roughly 1 MeV.

For disassembly by molecular dynamics we approximate the nuclear part of the force by a well-known parametrisation [16]:

$$v(r) = \begin{cases} A[B(r_0/r)^p - (r_0/r)^q] \exp[1/(r/r_0 - a)], & \text{for } r/r_0 < a \\ 0, & \text{for } r/r_0 \geq a \end{cases} \quad (1)$$

Here r_0 is the distance between the centres of two adjacent lattices. We have chosen $p = 2$, $q = 1$ and $a = 1.3$. The other constants A and B are chosen so that the potential acquires the prescribed value $-\epsilon$ at $r = r_0$. With this potential the interaction between two nucleons is zero when they are more than $1.3r_0$ apart and the interaction begins to become strongly repulsive for r significantly less than r_0 ; yet the potential is smooth enough that accurate numerical solutions of time evolution of nucleons can be obtained. The time evolution equations for each nucleon are, as usual, given by $\partial \mathbf{p}_i / \partial t = -\sum_{j \neq i} \nabla_i v(r_{ij})$ and $\partial \mathbf{r}_i / \partial t = \mathbf{p}_i / m$.

The lattice gas predictions for cluster production can only be calculated for the case where the Coulomb interaction is not explicitly included but only through a lower value of ϵ . As mentioned already the cluster distribution is calculated immediately after initialisation. The lattice filling is done and the momenta are then generated from a Monte-Carlo sampling of a Maxwell-Boltzmann distribution with a prescribed temperature. Nucleons in two neighbouring cells are considered to be part of the same cluster if the kinetic energy of relative motion is not large enough to overcome the attractive interaction, i. e., $p_r^2/2\mu - \epsilon < 0$. Here μ is the reduced mass and is equal to $m/2$. This definition is the simplest that one can provide and is physically reasonable. It should be emphasized that it is by no means a unique one. The prescription manages to reduce a many body problem of cluster production into a sum of independent two body problems. One can easily construct scenarios where this prescription may underestimate the size of a cluster and scenarios where this prescription may overestimate the size of a cluster. It should be pointed out that this formula for bond formation has the same structure as the one used in [6]. Since each particle obeys the Maxwell-Boltzmann distribution, the distribution of relative momentum between two

particles is also a Maxwell-Boltzmann, i.e., $P(\mathbf{p}_r) = [1/(2\pi\mu kT)^{3/2}] \exp[-\mathbf{p}_r^2/2\mu kT]$. We can then write down a formula for the bonding probability which is temperature dependent

$$p = 1 - \frac{4\pi}{(2\pi\mu kT)^{3/2}} \int_{\sqrt{2\mu\epsilon}}^{\infty} e^{-\mathbf{p}_r^2/2\mu kT} p_r^2 dp_r \quad (2)$$

Switching to a variable $E = p_r^2/2\mu$ we get

$$p = 1 - \frac{\int_{\epsilon}^{\infty} e^{-E/kT} E^{1/2} dE}{\int_0^{\infty} e^{-E/kT} E^{1/2} dE} \quad (3)$$

which is identical with the formula of [6].

For molecular dynamics calculation after initialisation we do the time propagation long enough so that for cluster production the asymptotic time has been reached. Two nucleons are part of the same cluster if the configuration distance between them is less than $1.3r_0$. We stop the calculation after the original blob of matter has expanded to 64 times its volume at initialisation. For low temperature this means doing the time evolution as long as 1000 fm/c. We use a time step of 0.1 fm/c and update positions and momenta half a time step apart ("leap frog" method). The energy conservation in our calculation is accurate to within 1 one percent. The program conserves total momentum identically. Below we now consider specific cases.

III. RESULTS

In Ref. [1] we found that a freeze-out density $\rho = .39\rho_0$ gave the best fit with data. Here we present data with this freeze-out density. A few calculations with a higher value of freeze-out density were also performed but only to ascertain that the trends of the results are not strongly dependent on the freeze-out density employed.

Fig. 1 shows the results of a $Y(A)$ - A plot of a lattice gas calculation. This is a repeat of the type of calculation done in [1,2]. The value of ϵ used is 3.7 MeV. This curve should be compared with a molecular dynamics calculation shown in Fig. 2. This calculation uses the same ϵ and no explicit Coulomb interaction. The similarity between Figs. 1 and 2 is

quite striking and leads us to conclude that the simple prescription of cluster counting is very reasonable. In Fig. 3 we have done a molecular dynamics calculation where we explicitly put in the Coulomb interaction. Accordingly the value of ϵ has been increased from 3.7 MeV to 4.7 MeV. There are now some changes from the results of Figs. 1 and 2, but not a great deal. Specially the deduced value of the slope τ is again the lowest at $T = T_c$ and rises both below and above this temperature. T_c is 1.1275ϵ and is the critical temperature in the lattice gas model. The results for τ are summarised in Fig. 4 where it is seen that the explicit inclusion of the Coulomb interaction has not modified the predominant characteristics observed in calculations without explicit inclusion of the Coulomb interaction. Here τ was obtained from linear fits of fragmentation distributions in $\log Y(A)$ *vs* $\log A$ plots. That is, τ is determined by minimizing the χ^2 defined as:

$$\chi^2 = \sum_i (F(A_i) - F_i)^2. \quad (4)$$

Here $F(A_i) \equiv \log Y(A_i) = \text{const} - \tau \log A_i$ is the fitted yield for fragment of size A_i , and $F_i \equiv \log Y_i$ is the corresponding simulated yield. To maintain sufficient statistics and to exclude the largest cluster, only fragments of sizes between 1 and 12 were used. In Fig. 5 for completeness we have shown a $Y(Z)$ against Z curve. This is the type of curve that are typically presented as experimental results.

Figs 6, 7 and 8 give our results for Au on Au. We plot both $Y(A)$ against A and $Y(Z)$ against Z . For molecular dynamics without explicit inclusion of the Coulomb interaction we have used $\epsilon = 3.7$ MeV and for calculation with explicit inclusion of the Coulomb interaction we have used $\epsilon = 4.7$ MeV. However now the results are very different for the two cases. In one (Fig. 6) there is a minimum in τ at $T = T_c$. A second spike at $T = 0.4T_c$ is indicative of a percolating cluster. In Fig. 7 with explicit inclusion of the Coulomb interaction, the percolating cluster has disappeared. We also see that below the critical temperature the τ values from the two calculations begin to diverge. With Coulomb explicitly included the minimum in τ has disappeared and one can get a value of τ much less than 2. These results are summarised in Fig. 8. Our results are in qualitative agreement with the experimental

results for Au on Au. Experimental results are given as a function of the beam energy and thus we need a conversion from temperature to beam energy. This conversion needs to be done carefully because at initialisation, which is the starting point of our calculation we can expect that some energy is already in collective motion and does not appear as thermal excitation. The model does not include this aspect. In Ref. [1] a phenomenological mapping of temperature to beam energy was deduced from [6]. As an estimate only if we assume that at the initial time $3/8$ of the initial energy is stored in collective motion then a beam energy of 35MeV/nucleon would correspond to $0.3T_c$. Our calculated value of τ is then 1.4 compared to the experimental value of 1.25 [10]. As in experimental data the calculated $Y(A)$ against A deviates from a power law with higher excitation energy. We nonetheless deduce a effective value of τ from a very approximate fit and these are shown in Fig. 8. We regard τ as a measure of global feature of $Y(A)$, although power-law fits are poor at high temperatures. To maintain sufficient statistics, we used fragments of size between 1 and 20 for high temperatures ($T \geq T_c$) when heavier fragments are rare. For low temperatures ($T < T_c$) larger fragments were also included. Our calculation at about $1.1T_c$ fits the data for beam energy 100 MeV/nucleon. For the calculation with Coulomb interaction included we use T_c merely as an energy scale; there is no implication that T_c is the critical temperature of the system. The principal point we want to emphasize is that we have reproduced the most significant features of the data for Au on Au as contrasted with those for Ar on Sc, namely that in the former case there is no minimum in the value of τ and that the value of τ can be significantly below 2.

IV. CONCLUSION

This problem started out as an effort to understand why the fragmentation data for Au on Au are so different from that of Ar on Sc and if the data totally ruin all validity of the simple concepts used in the lattice gas model. The calculation done here suggests that the lattice gas model is reasonable for medium mass collisions; it probably would have been as

valid for collisions of very large masses but for the very large Coulomb force which begins to make its presence felt and destroys the simple predictions. It has often been assumed that the larger the system of colliding nuclei the better is the chance of learning about phase transition in nuclear matter. However larger colliding masses also bring in much larger Coulomb forces and it will be necessary to take into account of the Coulomb effects before the signals for phase transitions can be understood. With large masses the mean field of the protons are very different from that of the neutrons and theories must be able to treat them differentially. There clearly are needs for simple theories which are able to handle this difference.

ACKNOWLEDGMENTS

We are very grateful to Miniball Group of Michigan State University for providing with recent experimental results for central Au on Au collisions. This work was supported in part by the Natural Sciences and Engineering Research Council of Canada and by the FCAR fund of the Québec Government.

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FIGURE CAPTIONS

Fig. 1 The mass yield distributions obtained from the lattice gas model for lattice $N = 6^3$ and $n = 85$, at temperatures $T/T_C = 0.5, 1.0$ and 1.5 . Here $T_C = 1.1275\epsilon$ is the thermal critical temperature.

Fig. 2 The mass yield distributions obtained from molecular dynamics calculations without the inclusion of Coulomb interaction. The lattice size, number of nucleons and temperatures are the same for the corresponding curves in Fig. 1.

Fig. 3 The same as Fig. 2, but the Coulomb interaction is taken into account.

Fig. 4 The value of τ obtained from lattice gas model and molecular dynamics calculations are plotted as a function of temperature for $N = 6^3$ and $n = 85$.

Fig. 5 The charge yield distributions obtained from the molecular dynamics calculation with Coulomb interaction are shown.

Fig. 6 The mass and charge yield distributions for Au on Au collisions obtained from the molecular dynamics without Coulomb interaction.

Fig. 7 The same as Fig. 6, but with Coulomb interaction.

Fig. 8 The value of τ in Au on Au collisions obtained from molecular dynamics calculations with and without Coulomb interaction are plotted as a function of temperature.

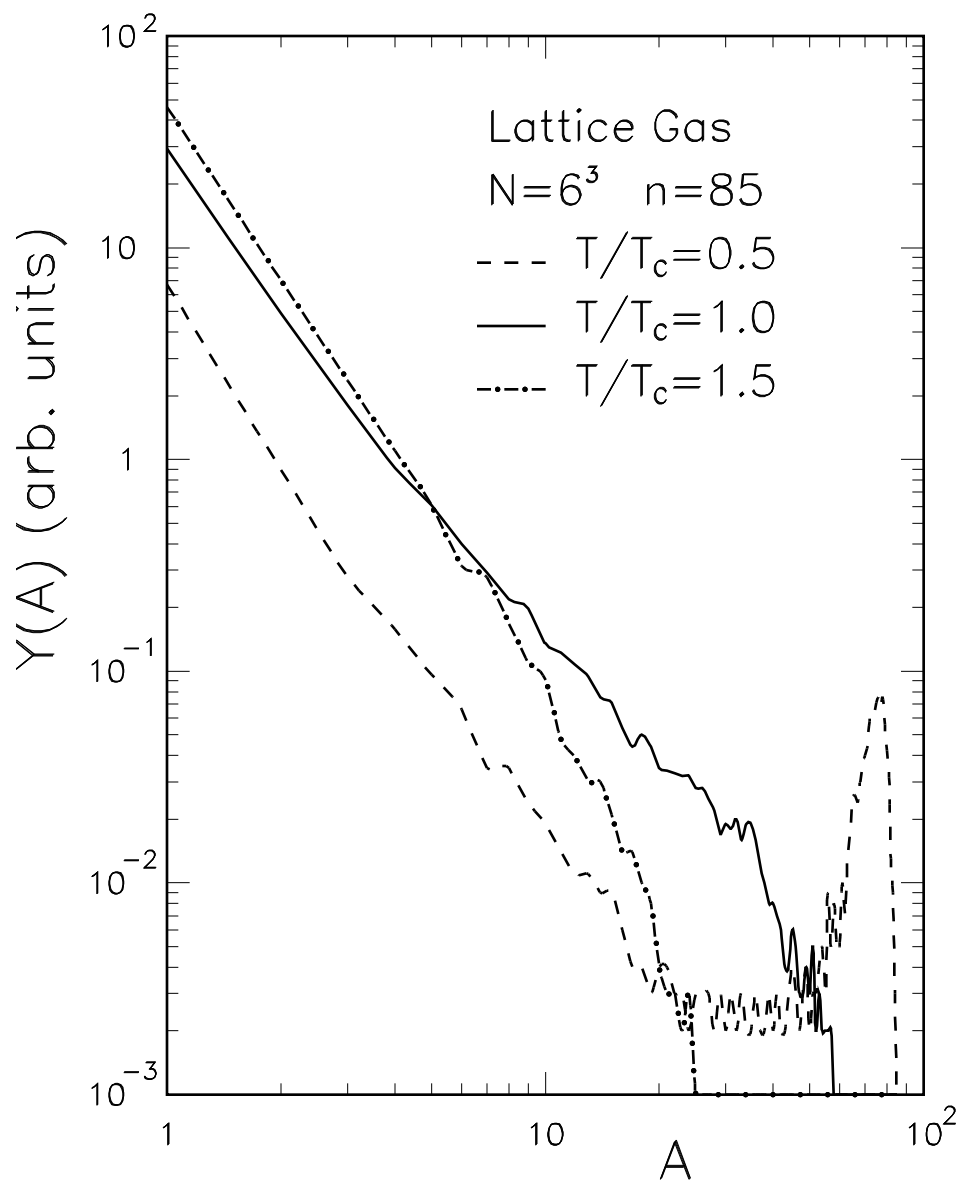


Fig. 1

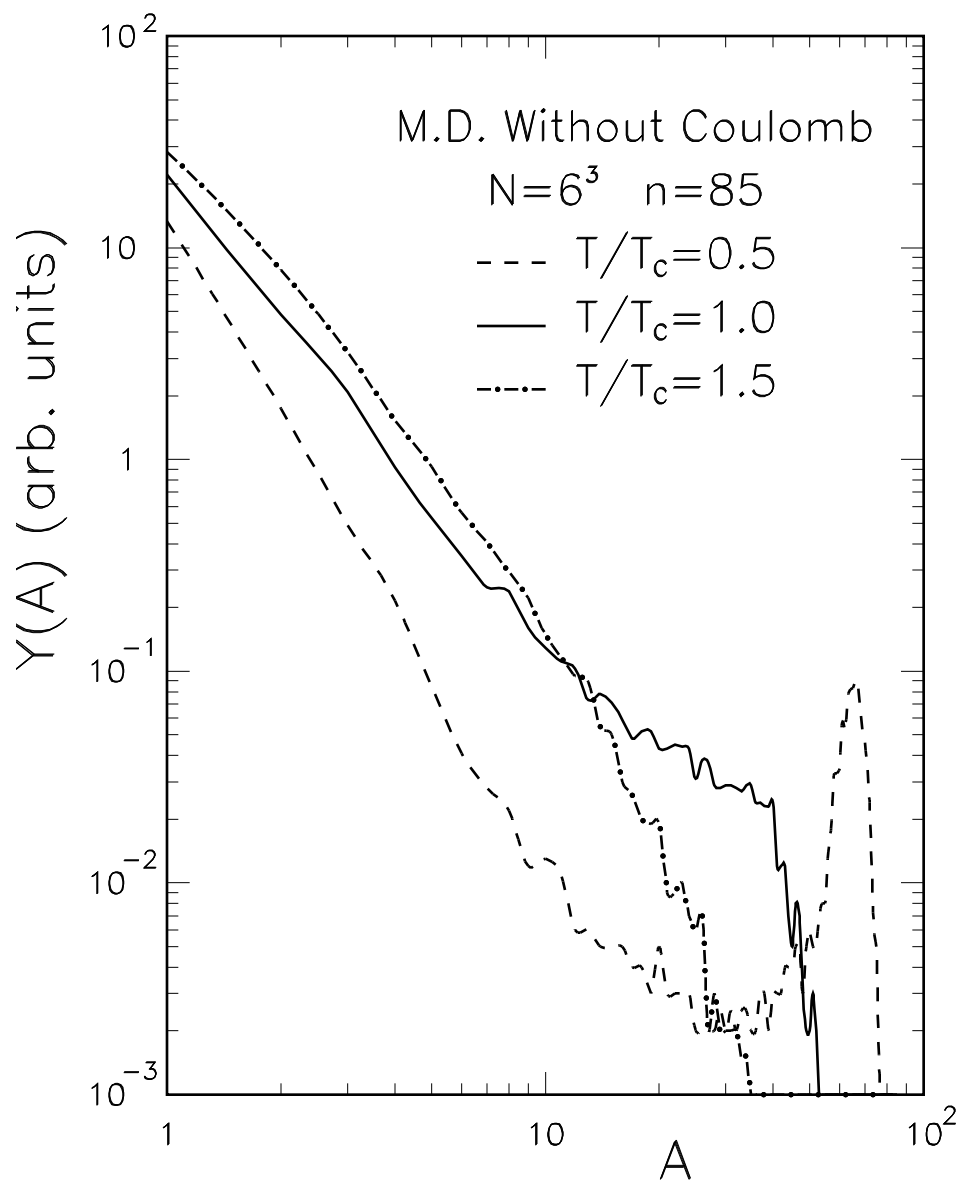


Fig. 2

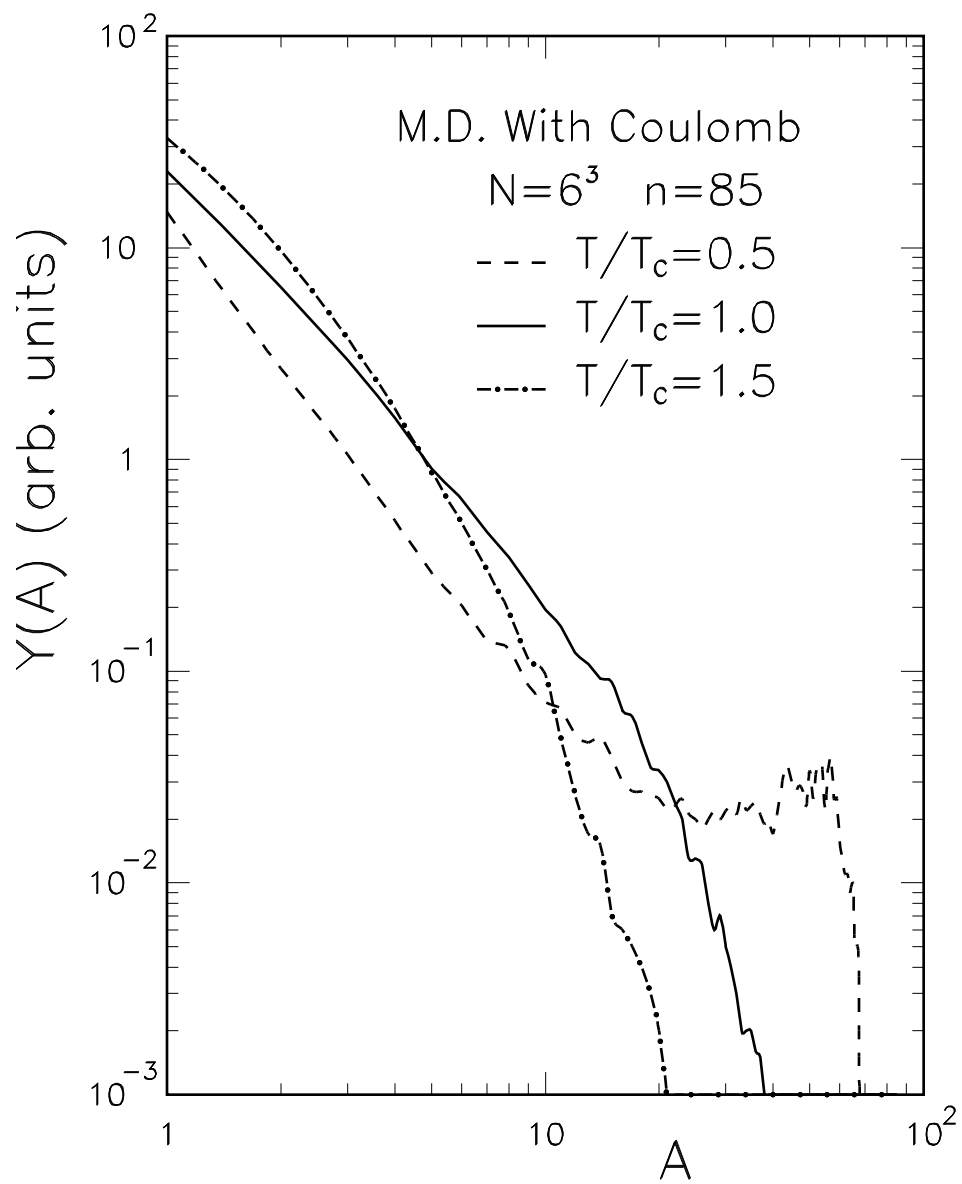


Fig. 3

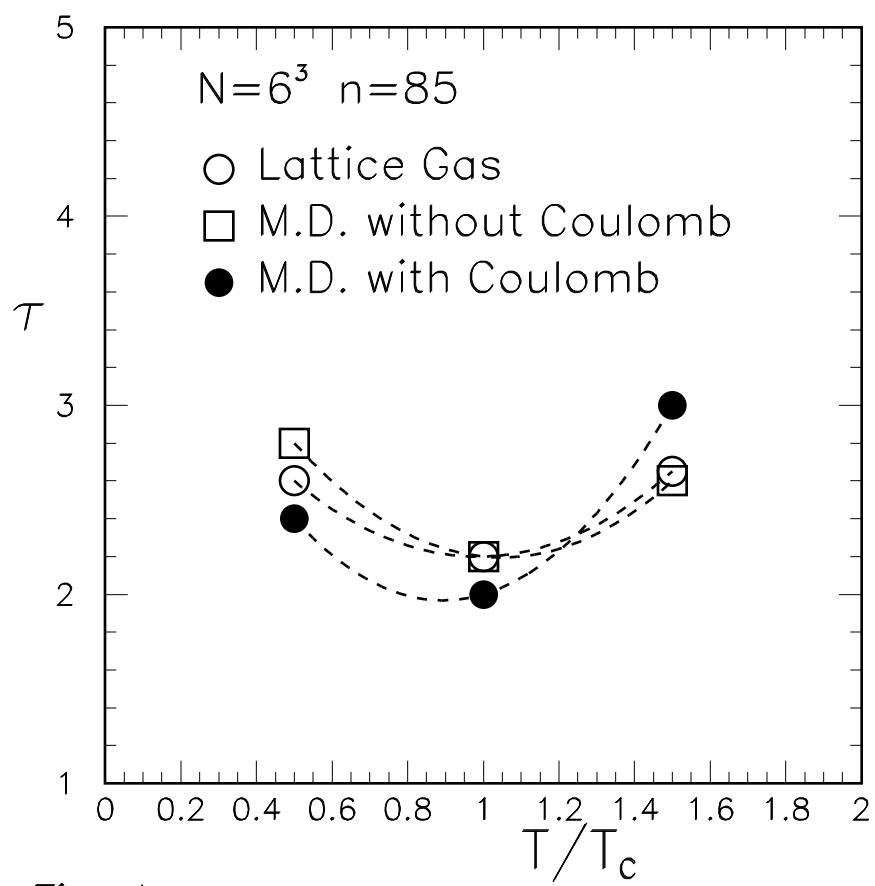


Fig. 4

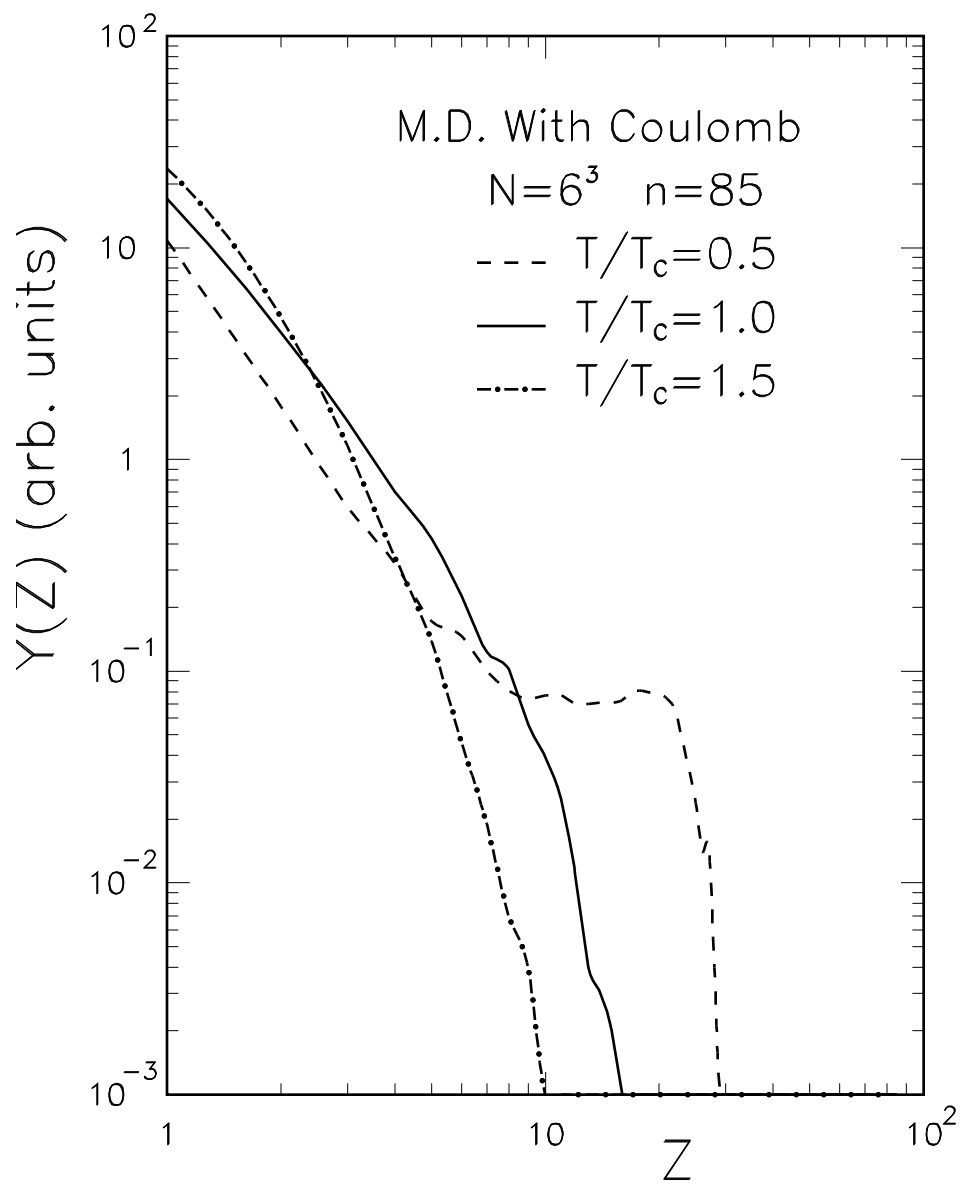


Fig. 5

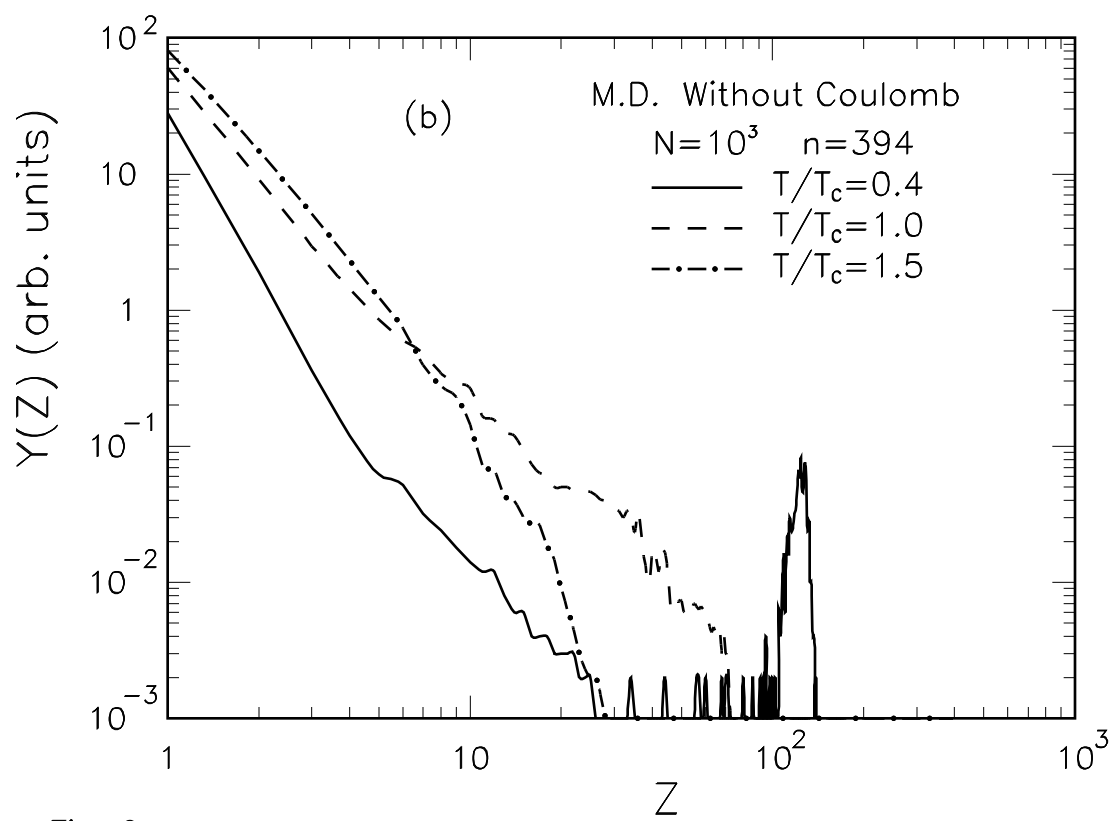
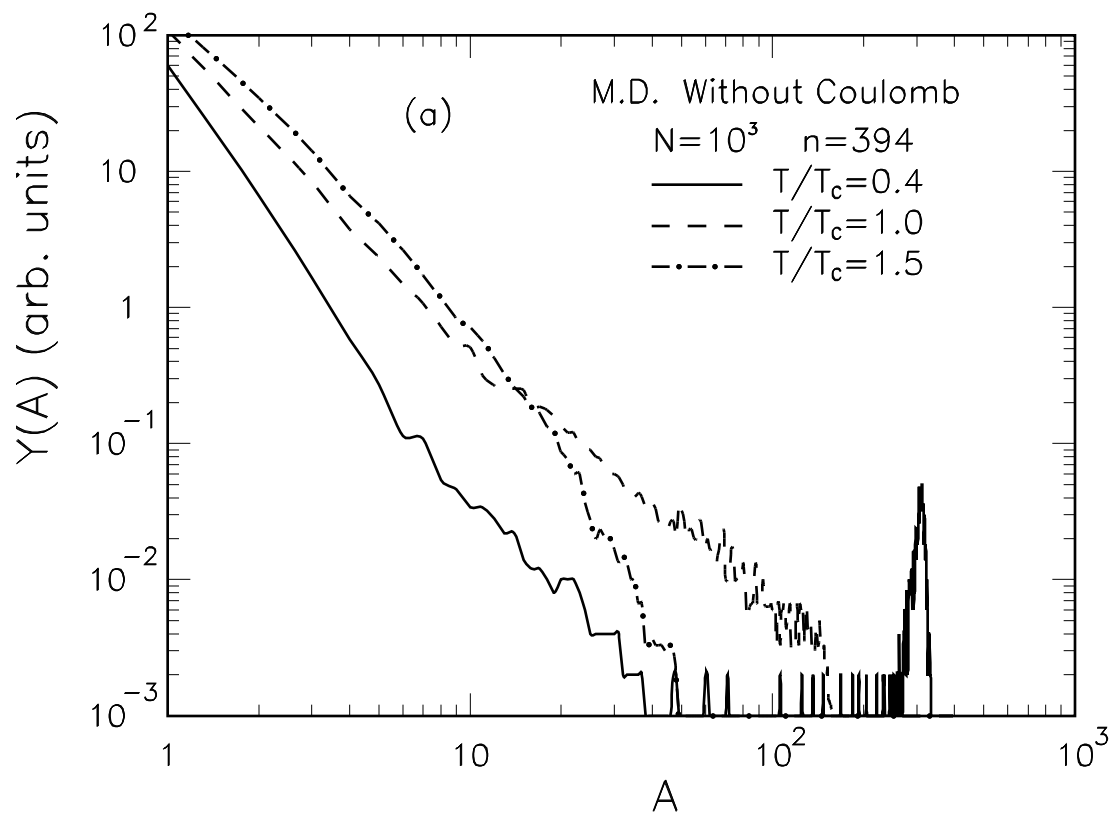


Fig. 6

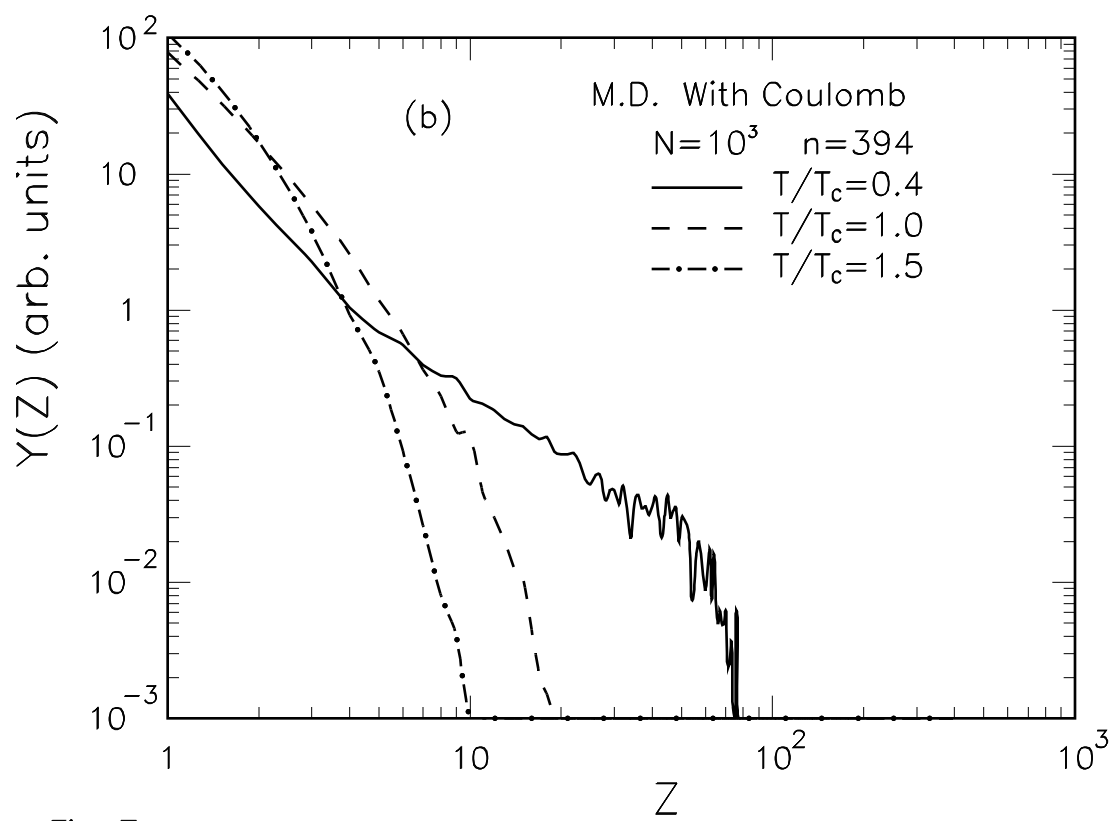
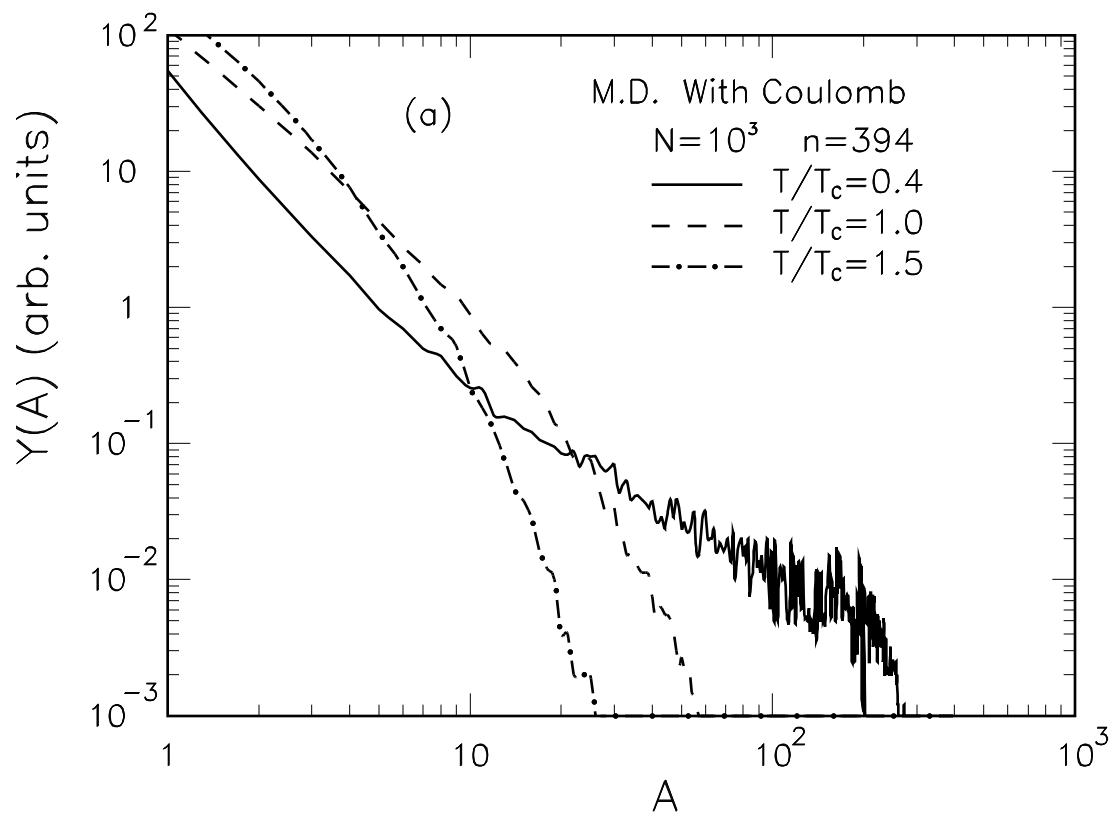


Fig. 7

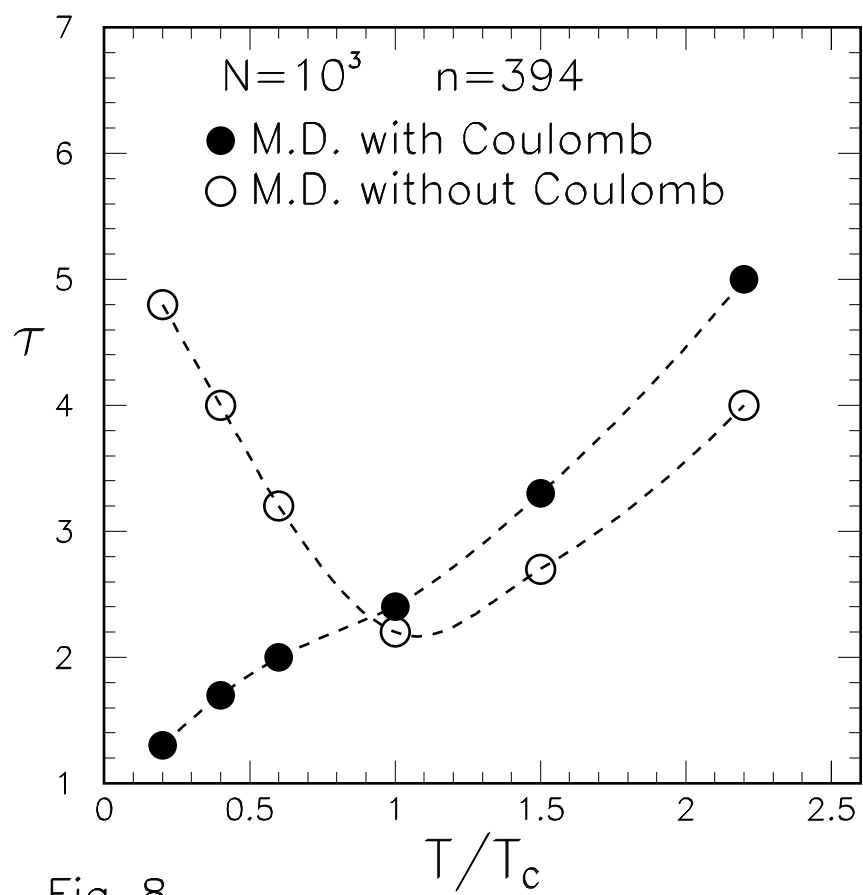


Fig. 8